



DD2434 – Advanced Machine Learning

Lecture 3: **Linear regression, model comparison**

Pawel Herman

Computational Science and Technology (CST)

KTH Royal Institute of Technology

November 2018

- Recap
- Regression models
- Model selection

Short outline for today

1. Recap from Lecture 2
2. Regression models
 - a) maximum likelihood, regularization
 - b) Bayesian approach
3. Model selection.

- **Recap**
- Regression models
- Model selection

- **Bayesian viewpoint**
- Learning and inference
- Model complexity and selection

Main points in lecture 2

- Motivation for a probabilistic perspective of machine learning
- Other flavours of ML theory (e.g. PAC)
- General philosophy of a Bayesian approach

$$p(\mathbf{w} \mid \mathcal{D}) = \frac{p(\mathcal{D} \mid \mathbf{w}) p(\mathbf{w})}{p(\mathcal{D})}$$

$$\text{posterior} \propto \text{likelihood} \times \text{prior}$$

- **Recap**
- Regression models
- Model selection

- **Bayesian viewpoint**
- Learning and inference
- Model complexity and selection

Main points in lecture 2

- Motivation for a probabilistic perspective of machine learning – scientific discipline
- General philosophy of a Bayesian approach
- **Bayesian vs frequentist viewpoint**

- **Recap**
- Regression models
- Model selection

- Bayesian viewpoint
- **Learning and inference**
- Model complexity and selection

Main points in lecture 2

- Motivation for a probabilistic perspective of machine learning – scientific discipline
- General philosophy of a Bayesian approach
- Bayesian vs frequentist viewpoint
- **Learning as inference, regression example**

Learning as inference – recap

1) **Maximise the likelihood**

$$\mathcal{D} \rightarrow \mathbf{w}_{\text{ML}} \quad \ln p(\mathbf{t} | \mathbf{X}, \mathbf{w}, \beta) = -\frac{\beta}{2} \sum_{n=1}^N \{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi)$$

2) Parameters of the model as random variables with a prior distribution

$$\mathcal{D}, p(\mathbf{w}) \rightarrow \mathbf{w}_{\text{MAP}} \quad p(\mathbf{w} | \alpha) = \mathcal{N}(\mathbf{w} | \mathbf{0}, \alpha^{-1} \mathbf{I})$$

Maximise the posterior: $\max p(\mathbf{w} | \mathbf{X}, \mathbf{t}, \alpha, \beta) \propto p(\mathbf{t} | \mathbf{X}, \mathbf{w}, \beta) p(\mathbf{w} | \alpha)$

3) **Marginalise** over parameters

Bayes: $\mathcal{D}, p(\mathbf{w}) \rightarrow p(\mathbf{w} | \mathcal{D})$

$$p(t | x, \mathbf{X}, \mathbf{t}) = \int p(t | x, \mathbf{w}, \beta) p(\mathbf{w} | \mathbf{X}, \mathbf{t}, \alpha, \beta) d\mathbf{w}$$

- **Recap**
- Regression models
- Model selection


- Bayesian viewpoint
- **Learning and inference**
- Model complexity and selection

Learning as inference – recap

1) $\mathcal{D} \rightarrow \mathbf{w}_{\text{ML}}$

2) $\mathcal{D}, p(\mathbf{w}) \rightarrow \mathbf{w}_{\text{MAP}}$

3) Bayes: $\mathcal{D}, p(\mathbf{w}) \rightarrow p(\mathbf{w} | \mathcal{D})$



We will elaborate more particularly on the Bayesian regression in this lecture.

- **Recap**
- Regression models
- Model selection

- Bayesian viewpoint
- Learning and inference
- Model complexity and selection

Main points in lecture 2

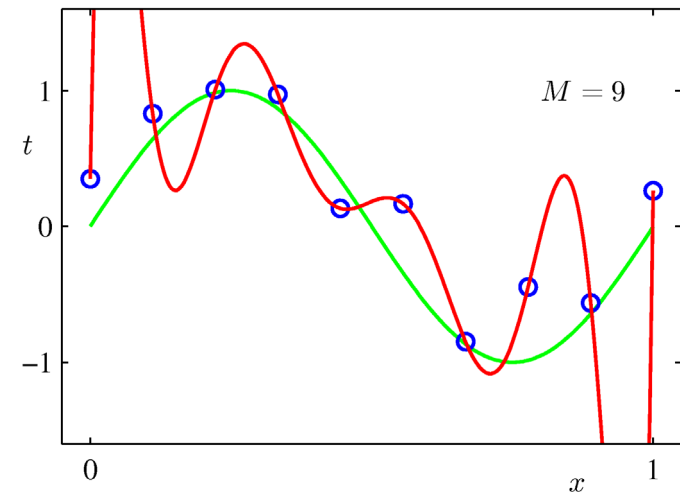
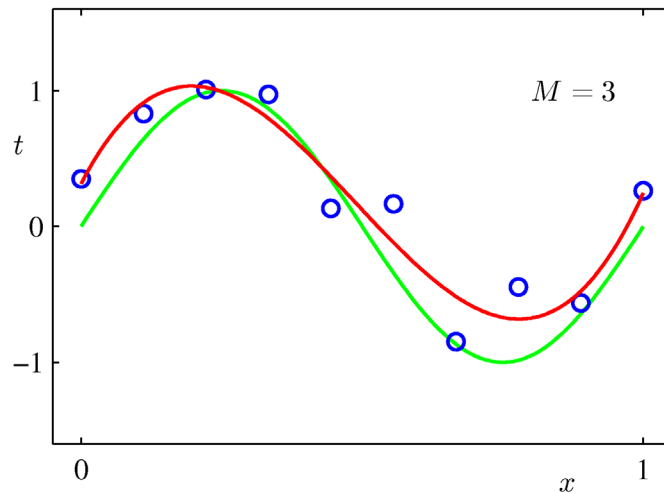
- Motivation for a probabilistic perspective of machine learning – scientific discipline
- General philosophy of a Bayesian approach
- Bayesian vs frequentist viewpoint
- Learning as inference, regression example
- Generative vs discriminative models
- Model complexity, overfitting, model selection

- **Recap**
- Regression models
- Model selection

- Bayesian viewpoint
- Learning and inference
- **Model complexity and selection**

Model complexity

- Overfitting of maximum likelihood models

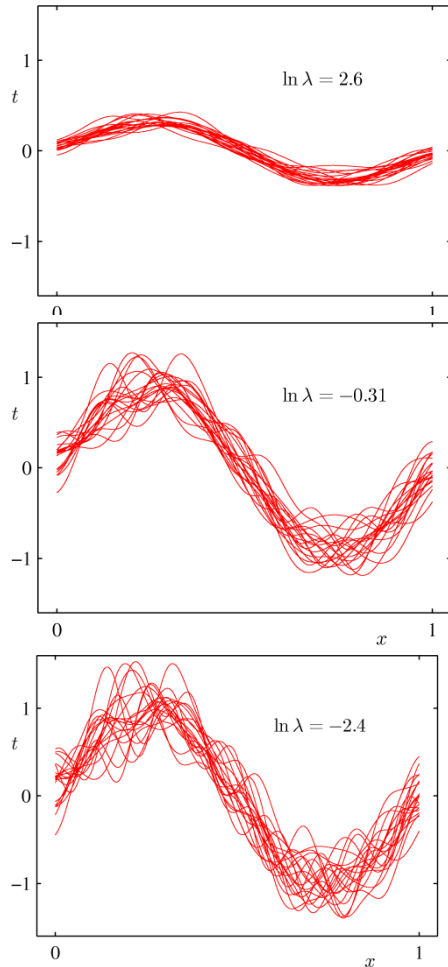


- **Recap**
- Regression models
- Model selection

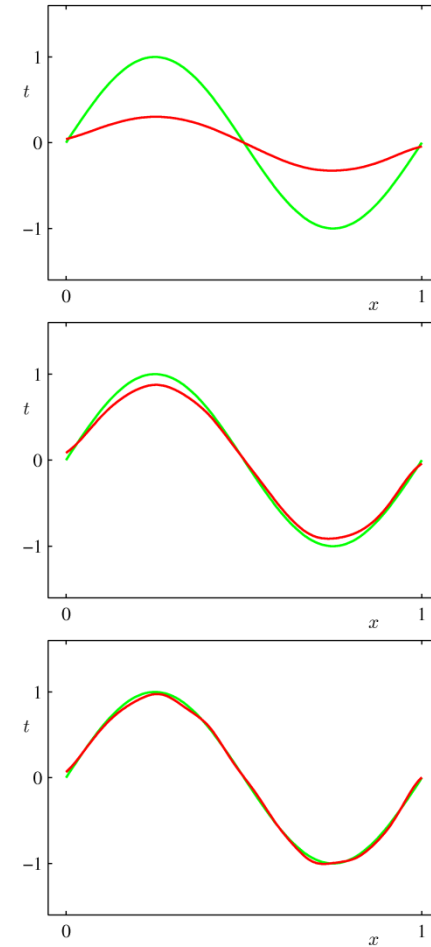
- Bayesian viewpoint
- Learning and inference
- **Model complexity and selection**

Bias-variance dilemma: model complexity

Models for different data samples



increased model complexity



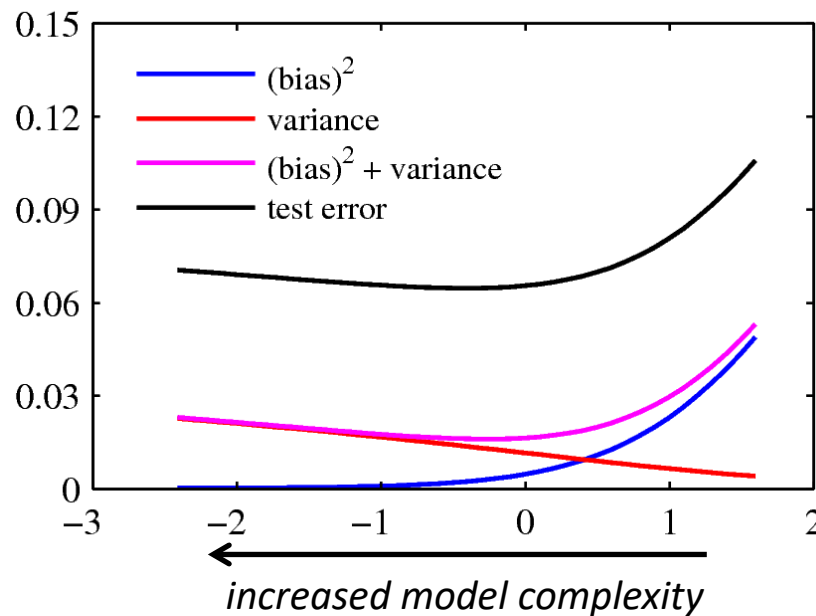
Model **average** and the **original**

- **Recap**
- Regression models
- Model selection

- Bayesian viewpoint
- Learning and inference
- **Model complexity and selection**

Bias-variance dilemma: model complexity

$$E[L] = (\text{bias})^2 + \text{variance} + \text{noise}$$



Model selection

- Occam's razor – *“Accept the simplest explanation that fits the data.”*
- Frequentist approach with maximum likelihood
 - bias-variance dilemma
 - need to control the model's complexity
 - regularisation
 - correction for the bias of ML estimates (AIC, BIC)
 - empirical estimate of generalisation error on a hold-out set (validation, resampling)
 - structural risk minimization (SRM) (minimise upper bound on the true risk), see also VC dimension (statistical learning theory)

- Recap
- **Regression models**
- Model selection

Short outline for today

1. Recap from Lecture 2
2. Regression models
 - a) maximum likelihood, regularization
 - b) Bayesian approach, model selection
3. Model selection.

Linear regression – the “*work horse*” of ML

- Linear basis function models

$$y(\mathbf{x}, \mathbf{w}) = \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x})$$

$$\mathbf{w} = (w_0, \dots, w_{M-1})^T \quad \boldsymbol{\phi} = (\phi_0, \dots, \phi_{M-1})^T$$

e.g., for polynomial one-dimensional regression basis functions are $\phi_j(x) = x^j$

Linear regression – the “*work horse*” of ML

- Linear basis function models

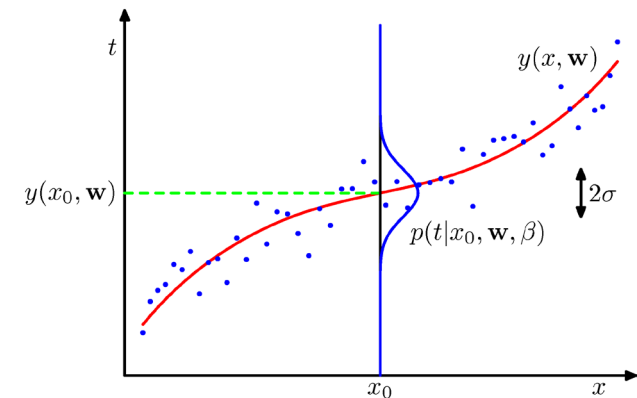
$$y(\mathbf{x}, \mathbf{w}) = \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x})$$

$$\mathbf{w} = (w_0, \dots, w_{M-1})^T \quad \boldsymbol{\phi} = (\phi_0, \dots, \phi_{M-1})^T$$

e.g., for polynomial one-dimensional regression basis functions are $\phi_j(x) = x^j$

$$t = y(\mathbf{x}, \mathbf{w}) + \varepsilon = \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}) + \varepsilon$$

$$p(t | \mathbf{x}, \mathbf{w}, \beta) = \mathcal{N}(t | y(\mathbf{x}, \mathbf{w}), \beta^{-1})$$



Linear regression

- Maximum likelihood estimation

$$y(\mathbf{x}, \mathbf{w}) = \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x})$$

Likelihood:

$$p(\mathbf{t}_{\mathcal{D}_{trn}} | \mathbf{X}_{\mathcal{D}_{trn}}, \mathbf{w}, \beta) = \prod_{n=1}^N \mathcal{N}(t_n | \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1})$$

$$\mathbf{X}_{\mathcal{D}_{trn}} = (\mathbf{x}_1, \dots, \mathbf{x}_N)$$

$$\mathbf{t}_{\mathcal{D}_{trn}} = (t_1, \dots, t_N)$$



$$\ln p(\mathbf{t}_{\mathcal{D}_{trn}} | \mathbf{X}_{\mathcal{D}_{trn}}, \mathbf{w}, \beta) = -\underbrace{\frac{\beta}{2} \sum_{n=1}^N \{t_n - \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n)\}^2}_{E_D(\mathbf{w})} + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi)$$

- Recap
- **Regression models**
- Kernel methods

- **Linear regression**
- Bayesian regression models
- Sequential Bayesian learning

Linear regression

- Maximum likelihood

$$0 = \sum_{n=1}^N t_n \phi(\mathbf{x}_n) - \mathbf{w}^T \left(\sum_{n=1}^N \phi(\mathbf{x}_n) \phi(\mathbf{x}_n)^T \right)$$

Linear regression

- Maximum likelihood

$$0 = \sum_{n=1}^N t_n \phi(\mathbf{x}_n) - \mathbf{w}^T \left(\sum_{n=1}^N \phi(\mathbf{x}_n) \phi(\mathbf{x}_n)^T \right)$$

Least-square solution:
(normal equations)

$$\mathbf{w}_{\text{ML}} = \left(\Phi^T \Phi \right)^{-1} \Phi^T \mathbf{t}$$

pseudo-inverse of
the design matrix Φ

$$\beta_{\text{ML}}^{-1} = \frac{1}{N} \sum_{n=1}^N \left\{ t_n - \mathbf{w}_{\text{ML}}^T \phi(\mathbf{x}_n) \right\}^2$$

Linear regression

- Maximum likelihood

$$0 = \sum_{n=1}^N t_n \phi(\mathbf{x}_n) - \mathbf{w}^T \left(\sum_{n=1}^N \phi(\mathbf{x}_n) \phi(\mathbf{x}_n)^T \right)$$

Least-square solution:
(normal equations)

$$\mathbf{w}_{\text{ML}} = \left(\Phi^T \Phi \right)^{-1} \Phi^T \mathbf{t}$$

pseudo-inverse of
the design matrix Φ

$$\Phi = \begin{pmatrix} \phi_0(\mathbf{x}_1) & \cdots & \phi_{M-1}(\mathbf{x}_1) \\ \vdots & \ddots & \vdots \\ \phi_0(\mathbf{x}_N) & \cdots & \phi_{M-1}(\mathbf{x}_N) \end{pmatrix}$$

Linear regression

- Maximum likelihood

$$0 = \sum_{n=1}^N t_n \phi(\mathbf{x}_n) - \mathbf{w}^T \left(\sum_{n=1}^N \phi(\mathbf{x}_n) \phi(\mathbf{x}_n)^T \right)$$

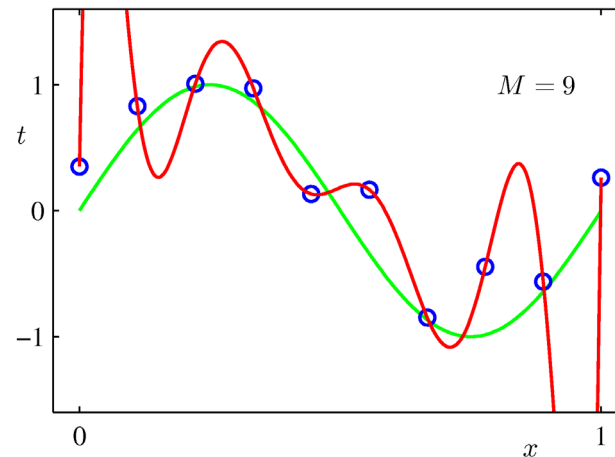
$$\begin{cases} \mathbf{w}_{\text{ML}} = (\Phi^T \Phi)^{-1} \Phi^T \mathbf{t} \\ \beta_{\text{ML}}^{-1} = \frac{1}{N} \sum_{n=1}^N \left\{ t_n - \mathbf{w}_{\text{ML}}^T \phi(\mathbf{x}_n) \right\}^2 \end{cases}$$

- Recap
- **Regression models**
- Kernel methods

- **Linear regression**
- Bayesian regression models
- Sequential Bayesian learning

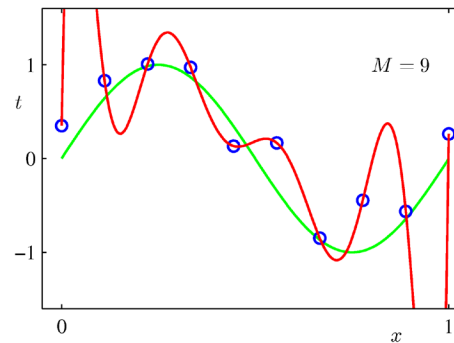
Linear regression - regularisation

- Problems with maximum likelihood estimate



Linear regression - regularisation

- Problems with maximum likelihood estimate



- We can address it by regularisation (parameter shrinkage)

$$\arg \min_{\mathbf{w}} \left\{ \frac{1}{2} \sum_{n=1}^N \{t_n - \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n)\}^2 + \frac{\lambda}{2} \mathbf{w}^T \mathbf{w} \right\} \quad (\text{weight decay})$$

$$\arg \min_{\mathbf{w}} \left\{ \frac{1}{2} \sum_{n=1}^N \{t_n - \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n)\}^2 + \frac{\lambda}{2} \sum_{j=1}^M |w_j|^q \right\} \quad (\text{lasso for } q=1)$$

Bayesian linear regression

- Bayesian treatment

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w} \mid \mathbf{m}_0, \mathbf{S}_0)$$

Bayesian linear regression

- Bayesian treatment

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w} \mid \mathbf{m}_0, \mathbf{S}_0)$$

For this **conjugate Gaussian prior** corresponding to the likelihood, the posterior has also Gaussian distribution:

$$p(\mathbf{w} \mid \mathbf{t}_{D_{trn}}) = \mathcal{N}(\mathbf{w} \mid \mathbf{m}_N, \mathbf{S}_N)$$

$$\mathbf{m}_N = \mathbf{S}_N \left(\mathbf{S}_0^{-1} \mathbf{m}_0 + \beta \Phi^T \mathbf{t}_{D_{trn}} \right)$$

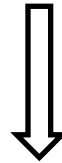
$$\mathbf{S}_N^{-1} = \mathbf{S}_0^{-1} + \beta \Phi^T \Phi$$

$$\Phi(\mathbf{X}_{D_{trn}}) \rightarrow \Phi$$

Bayesian linear regression

- Bayesian treatment

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w} \mid \mathbf{0}, \alpha^{-1} \mathbf{I})$$



$$p(\mathbf{w} \mid \mathbf{t}_{\mathcal{D}_{trn}}, \mathbf{X}_{\mathcal{D}_{trn}}, \alpha, \beta) = \mathcal{N}(\mathbf{w} \mid \mathbf{m}_N, \mathbf{S}_N)$$

$$\mathbf{m}_N = \beta \mathbf{S}_N \mathbf{\Phi}^T \mathbf{t}_{\mathcal{D}_{trn}}$$

$$\mathbf{S}_N^{-1} = \alpha \mathbf{I} + \beta \mathbf{\Phi}^T \mathbf{\Phi}$$

Bayesian linear regression

- Bayesian treatment

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w} \mid \mathbf{0}, \alpha^{-1} \mathbf{I})$$



the **likelihood part** of the log-posterior
dependent on \mathbf{w}

the **prior part** of the log-posterior
dependent on \mathbf{w}

log-posterior

$$\ln p(\mathbf{w} \mid \mathbf{t}_{\mathcal{D}_{trn}}, \mathbf{X}_{\mathcal{D}_{trn}}, \alpha, \beta) = \underbrace{-\frac{\beta}{2} \sum_{n=1}^N \{t_n - \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n)\}^2}_{\text{likelihood part}} \underbrace{-\frac{\alpha}{2} \mathbf{w}^T \mathbf{w}}_{\text{prior part}} + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi)$$

Bayesian linear regression

- Predictive distribution

$$\underbrace{p(t \mid \mathbf{x}, \mathbf{t}_{\mathcal{D}_{trn}}, \alpha, \beta)}_{\text{predictive}} = \int \underbrace{p(t \mid \mathbf{x}, \mathbf{w}, \beta)}_{\text{"noise" model}} \underbrace{p(\mathbf{w} \mid \mathbf{t}_{\mathcal{D}_{trn}}, \mathbf{X}_{\mathcal{D}_{trn}}, \alpha, \beta)}_{\text{posterior}} d\mathbf{w}$$

Bayesian linear regression

- Predictive distribution

$$\underbrace{p(t \mid \mathbf{x}, \mathbf{t}_{\mathcal{D}_{trn}}, \alpha, \beta)}_{\text{predictive}} = \int \underbrace{p(t \mid \mathbf{x}, \mathbf{w}, \beta)}_{\text{"noise" model}} \underbrace{p(\mathbf{w} \mid \mathbf{t}_{\mathcal{D}_{trn}}, \mathbf{X}_{\mathcal{D}_{trn}}, \alpha, \beta)}_{\text{posterior}} d\mathbf{w}$$

$$p(t \mid \mathbf{x}, \mathbf{t}_{\mathcal{D}_{trn}}, \alpha, \beta) = \mathcal{N}(t \mid \mathbf{m}_N^T \boldsymbol{\phi}(\mathbf{x}), \sigma_N^2(\mathbf{x}))$$

$$\mathbf{m}_N = \beta \mathbf{S}_N \boldsymbol{\Phi}^T \mathbf{t}_{\mathcal{D}_{trn}}$$

$$\mathbf{S}_N^{-1} = \alpha \mathbf{I} + \beta \boldsymbol{\Phi}^T \boldsymbol{\Phi}$$

$$\sigma_N^2(\mathbf{x}) = \frac{1}{\beta} + \boldsymbol{\phi}(\mathbf{x})^T \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x})$$

Bayesian linear regression

- Bayesian philosophy – overview

- in order to make predictions we need posterior

$$p(\mathbf{w} | \mathbf{t}, \mathbf{x})$$

- it can be updated (estimated) after the relevant information has been taken into account

Adapted from Carl Henrik Ek's lecture (DD2434, 2015)

Bayesian linear regression

- Bayesian philosophy

- in order to make predictions we need posterior

$$p(\mathbf{w} | \mathbf{t}, \mathbf{x})$$

- it can be updated (estimated) after the relevant information has been taken into account
- so, we need our **belief** about the model and the **observations** (data: \mathbf{t}, \mathbf{x})

Adapted from Carl Henrik Ek's lecture (DD2434, 2015)

Bayesian linear regression

- Bayesian philosophy

- in order to make predictions we need posterior

$$p(\mathbf{w} | \mathbf{t}, \mathbf{x})$$

- it can be updated (estimated) after the relevant information has been taken into account
- so, we need our belief about the model and the observations (data: \mathbf{t}, \mathbf{x})
- before we see the data, we express our **belief** about the regression params

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{0}, \alpha^{-1} \mathbf{I})$$

Adapted from Carl Henrik Ek's lecture (DD2434, 2015)

Bayesian linear regression

- Bayesian philosophy

- in order to make predictions we need posterior

$$p(\mathbf{w} | \mathbf{t}, \mathbf{x})$$

- it can be updated (estimated) after the relevant information has been taken into account
- so, we need our belief about the model and the observations (data: \mathbf{t}, \mathbf{x})
- before we see the data, we express our **belief** about the regression params

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{0}, \alpha^{-1} \mathbf{I})$$

very often we do not really
know too much in advance

Adapted from Carl Henrik Ek's lecture (DD2434, 2015)

Bayesian linear regression

- Bayesian philosophy (cont.)
 - how well does my model predicts (explains) data?
 - likelihood (like an error function) for a single sample n

$$p(t_n | \mathbf{w}, \mathbf{x}_n) = \mathcal{N}(t_n | \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1} \mathbf{I})$$

- if there is independence between samples, likelihood for all data \mathbf{t} amounts to

$$p(\mathbf{t} | \mathbf{w}, \mathbf{X}) = \prod_{n=1}^N \mathcal{N}(t_n | \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1} \mathbf{I})$$

Adapted from Carl Henrik Ek's lecture (DD2434, 2015)

Bayesian linear regression

- Bayesian philosophy – summary
 - The goal is to reach posterior distribution after all relevant information has been taken into account.
 - Prediction should reflect my beliefs in the model and the information in the observations.

Adapted from Carl Henrik Ek's lecture (DD2434, 2015)

Bayesian linear regression

- Bayesian philosophy – summary
 - The goal is to reach posterior distribution after all relevant information has been taken into account.
 - Prediction should reflect my beliefs in the model and the information in the observations.
 - So:
 - i. Choose a model
 - ii. Formulate prediction error by likelihood
 - iii. Formulate belief of a model in prior
 - iv. Marginalise irrelevant variables (parameters)

Adapted from Carl Henrik Ek's lecture (DD2434, 2015)

Bayesian linear regression

- Bayesian philosophy – summary
 - The goal is to reach posterior distribution after all relevant information has been taken into account.
 - Prediction should reflect my beliefs in the model and the information in the observations.
 - So:
 - i. Choose a model
 - ii. Formulate prediction error by likelihood
 - iii. Formulate belief of a model in prior
 - iv. Marginalise irrelevant variables (parameters)

Adapted from Carl Henrik Ek's lecture (DD2434, 2015)

Bayesian linear regression

- Bayesian philosophy – summary
 - The goal is to reach posterior distribution after all relevant information has been taken into account.
 - Prediction should reflect my beliefs in the model and the information in the observations.
 - So:

Gaussian distributions are *self-conjugate*, i.e.:

Gaussian prior + Gaussian likelihood → **Gaussian posterior**

Adapted from Carl Henrik Ek's lecture (DD2434, 2015)

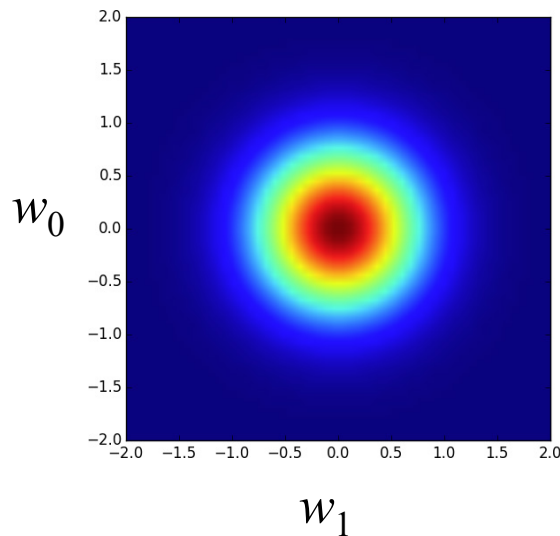
- Recap
- **Regression models**
- Kernel methods

- Linear regression
- Bayesian regression models
- **Sequential Bayesian learning**

Sequential Bayesian learning

$$y(x, \mathbf{w}) = -w_0 + w_1 x$$

$p(\mathbf{w})$



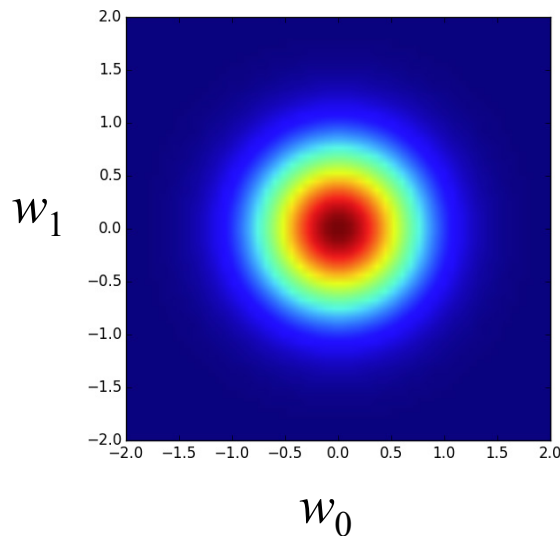
Adapted from Carl Henrik Ek's lecture (DD2434, 2015)

- Recap
- **Regression models**
- Kernel methods

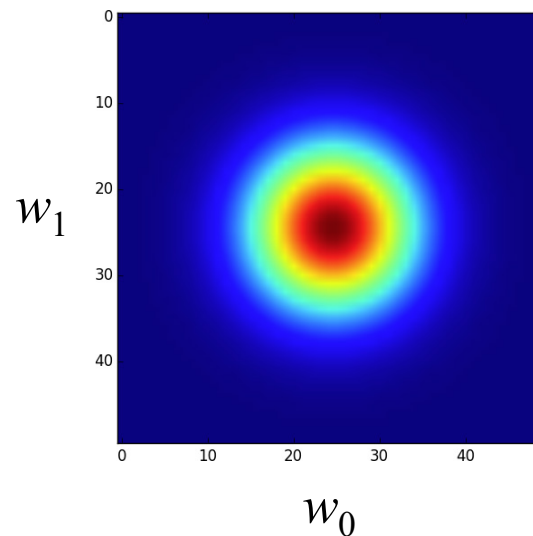
- Linear regression
- Bayesian regression models
- **Sequential Bayesian learning**

Sequential Bayesian learning

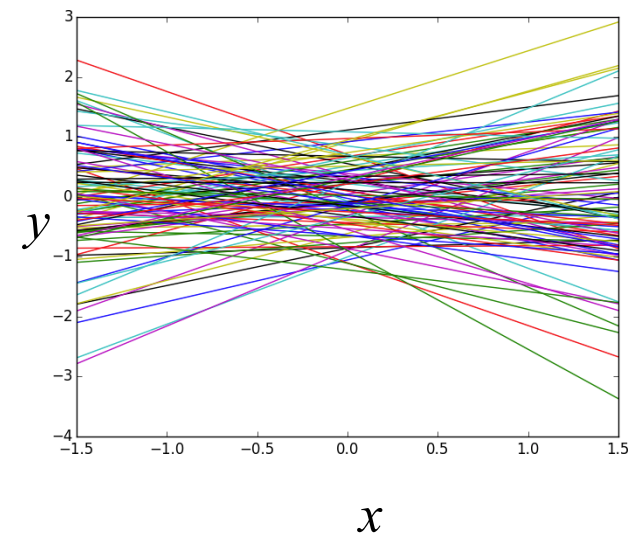
$p(\mathbf{w})$



$p(\mathbf{w} \mid x, y)$



\mathbf{w} samples in
data space (x, y)



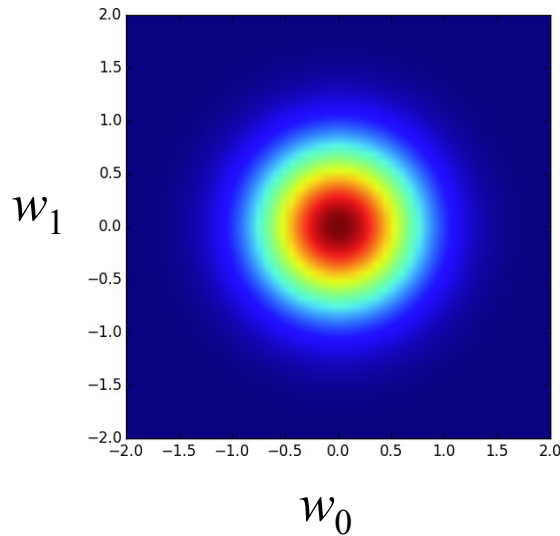
Adapted from Carl Henrik Ek's lecture (DD2434, 2015)

- Recap
- **Regression models**
- Kernel methods

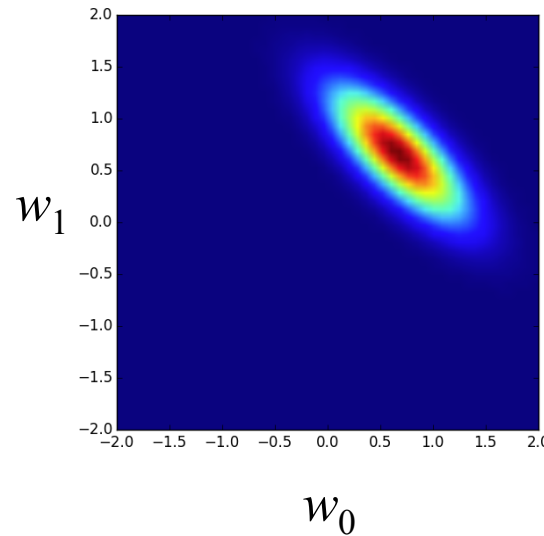
- Linear regression
- Bayesian regression models
- **Sequential Bayesian learning**

Sequential Bayesian learning

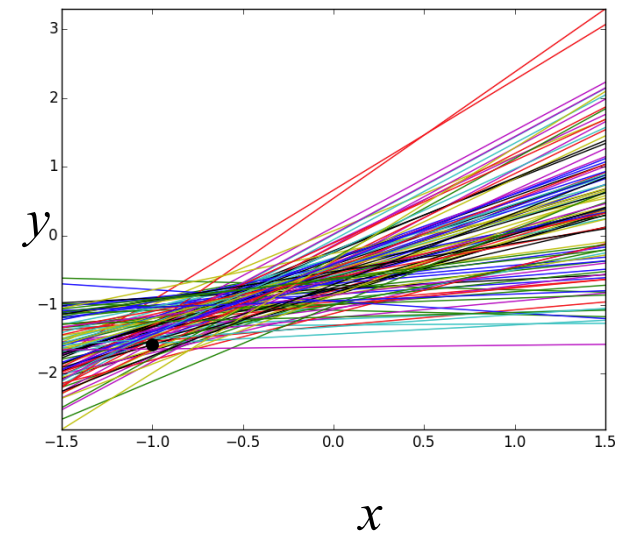
$$p(\mathbf{w})$$



$$p(\mathbf{w} \mid x, y)$$



\mathbf{w} samples in
data space (x, y)



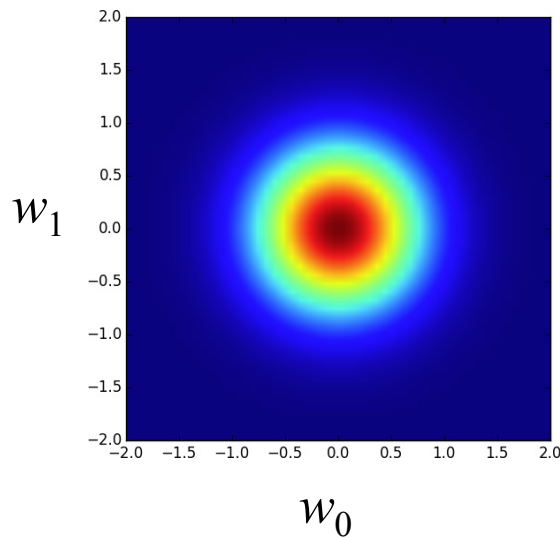
Adapted from Carl Henrik Ek's lecture (DD2434, 2015)

- Recap
- **Regression models**
- Kernel methods

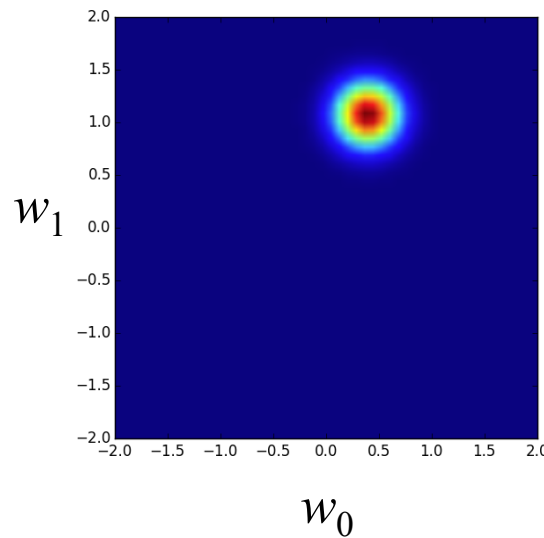
- Linear regression
- Bayesian regression models
- **Sequential Bayesian learning**

Sequential Bayesian learning

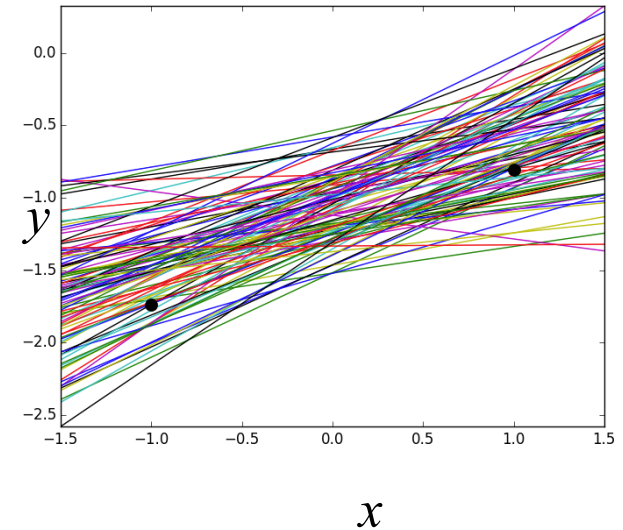
$$p(\mathbf{w})$$



$$p(\mathbf{w} \mid x, y)$$



\mathbf{w} samples in
data space (x, y)



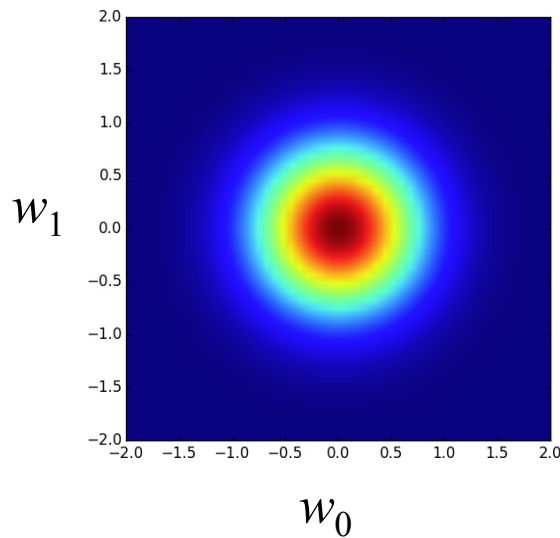
Adapted from Carl Henrik Ek's lecture (DD2434, 2015)

- Recap
- **Regression models**
- Kernel methods

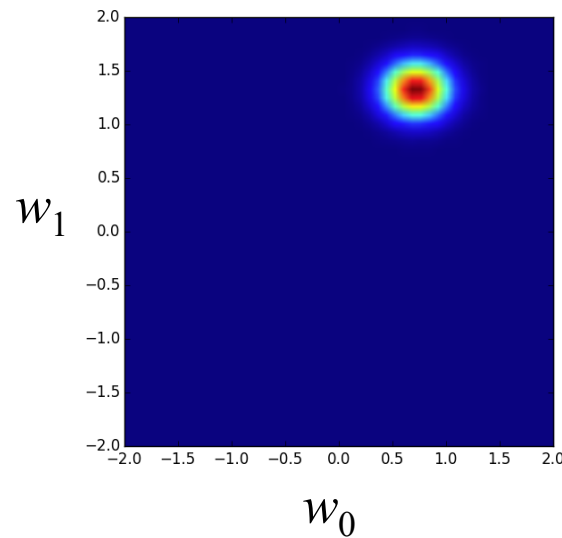
- Linear regression
- Bayesian regression models
- **Sequential Bayesian learning**

Sequential Bayesian learning

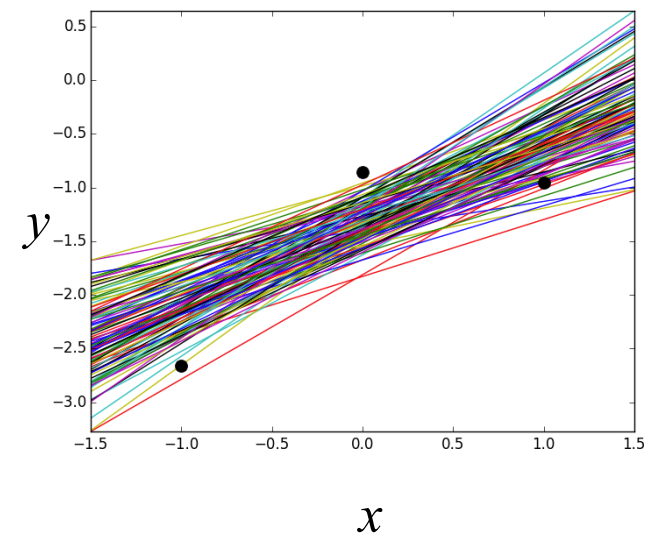
$$p(\mathbf{w})$$



$$p(\mathbf{w} \mid x, y)$$



\mathbf{w} samples in
data space (x, y)



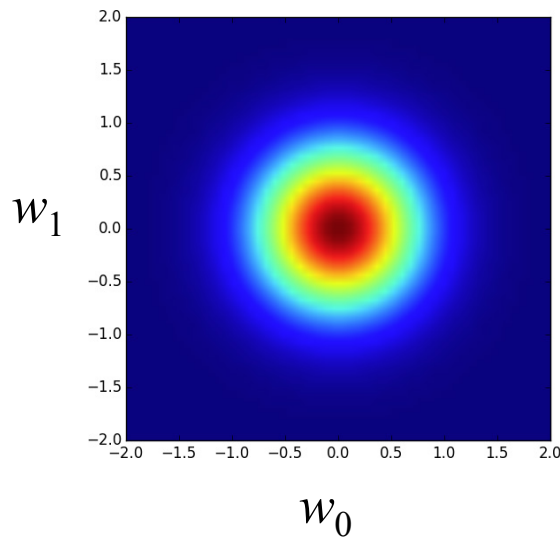
Adapted from Carl Henrik Ek's lecture (DD2434, 2015)

- Recap
- **Regression models**
- Kernel methods

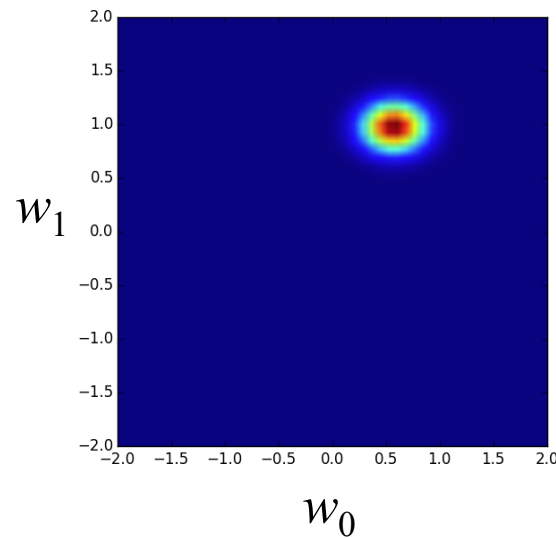
- Linear regression
- Bayesian regression models
- **Sequential Bayesian learning**

Sequential Bayesian learning

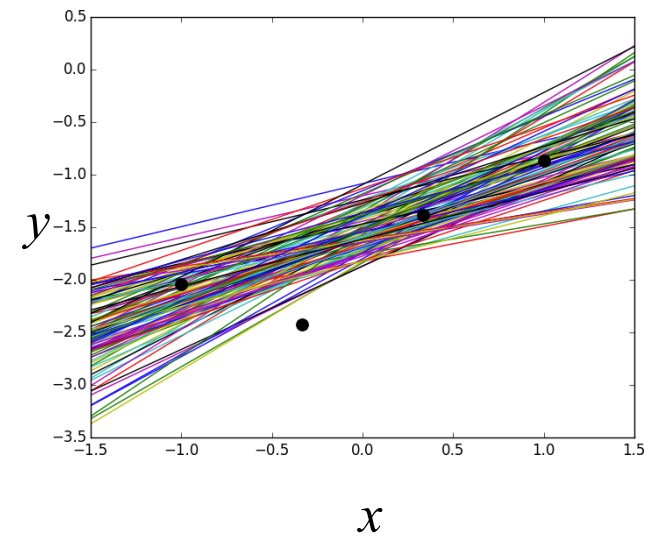
$$p(\mathbf{w})$$



$$p(\mathbf{w} \mid x, y)$$



\mathbf{w} samples in
data space (x, y)



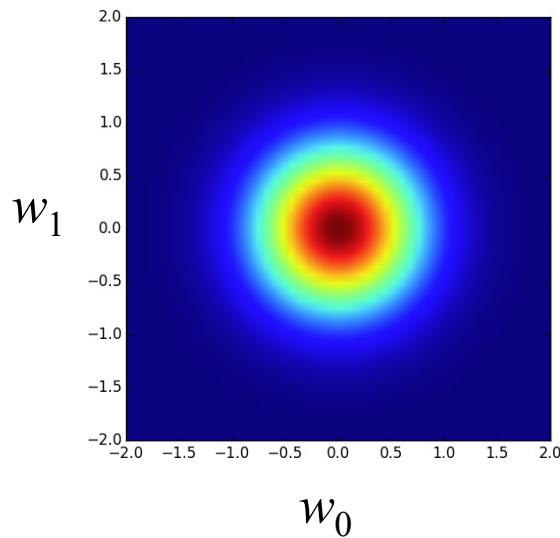
Adapted from Carl Henrik Ek's lecture (DD2434, 2015)

- Recap
- **Regression models**
- Kernel methods

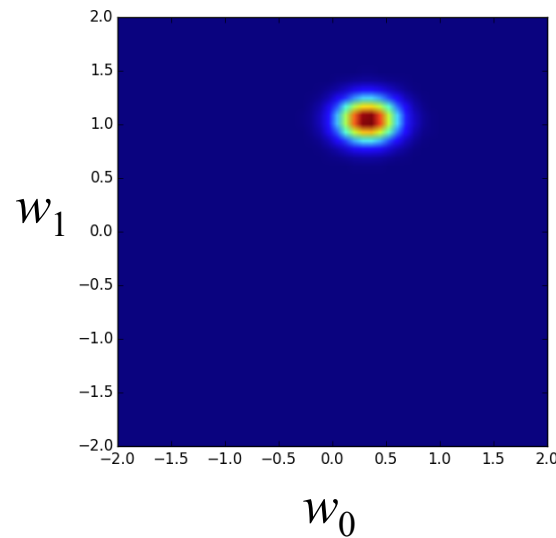
- Linear regression
- Bayesian regression models
- **Sequential Bayesian learning**

Sequential Bayesian learning

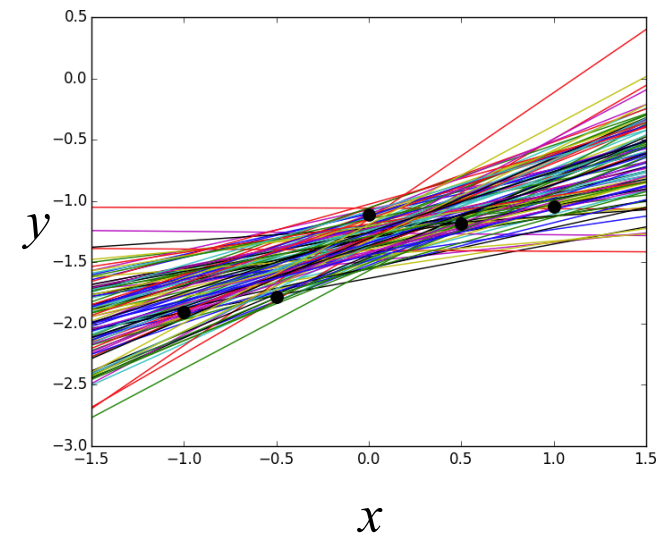
$$p(\mathbf{w})$$



$$p(\mathbf{w} \mid x, y)$$



\mathbf{w} samples in
data space (x, y)



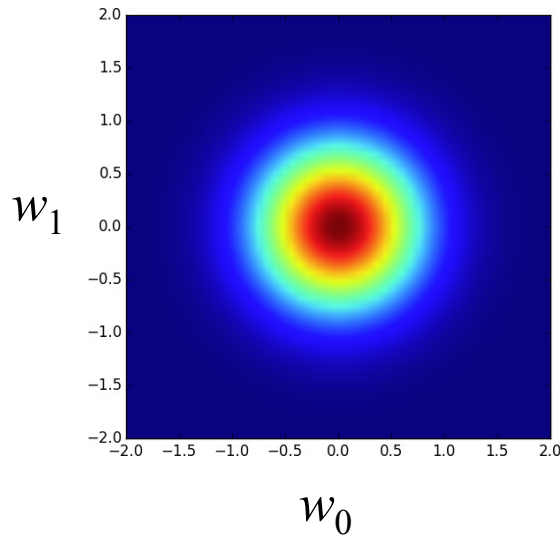
Adapted from Carl Henrik Ek's lecture (DD2434, 2015)

- Recap
- **Regression models**
- Kernel methods

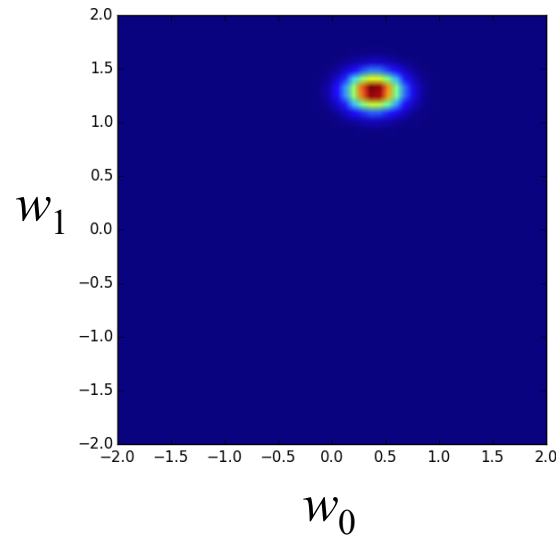
- Linear regression
- Bayesian regression models
- **Sequential Bayesian learning**

Sequential Bayesian learning

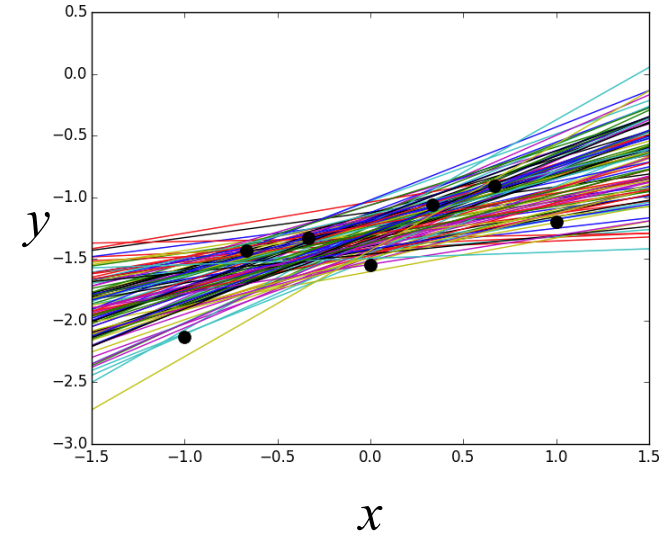
$$p(\mathbf{w})$$



$$p(\mathbf{w} \mid x, y)$$



\mathbf{w} samples in
data space (x, y)



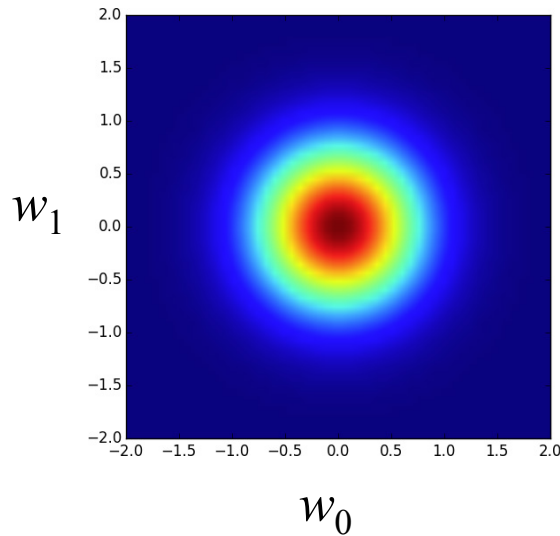
Adapted from Carl Henrik Ek's lecture (DD2434, 2015)

- Recap
- **Regression models**
- Kernel methods

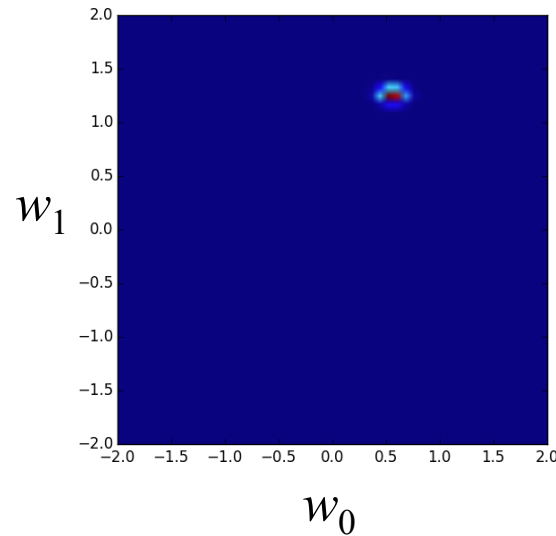
- Linear regression
- Bayesian regression models
- **Sequential Bayesian learning**

Sequential Bayesian learning

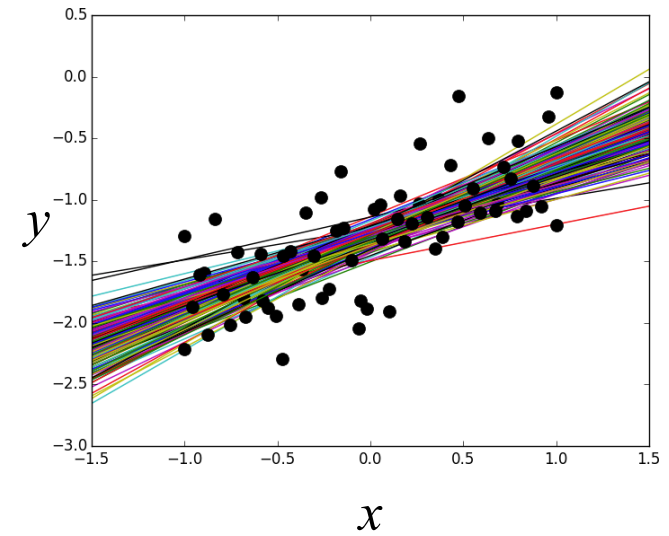
$$p(\mathbf{w})$$



$$p(\mathbf{w} \mid x, y)$$



\mathbf{w} samples in
data space (x, y)



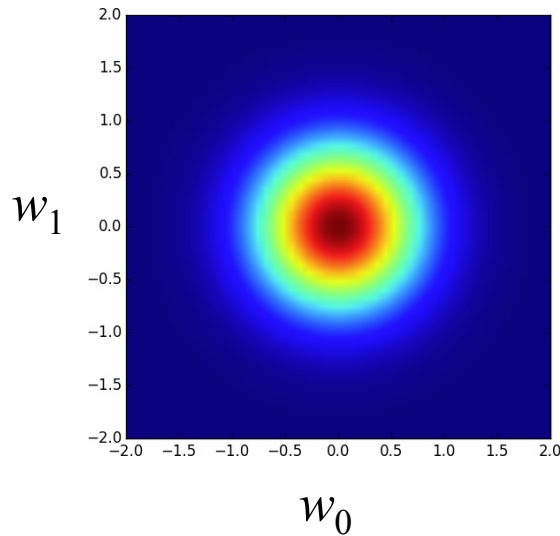
Adapted from Carl Henrik Ek's lecture (DD2434, 2015)

- Recap
- **Regression models**
- Kernel methods

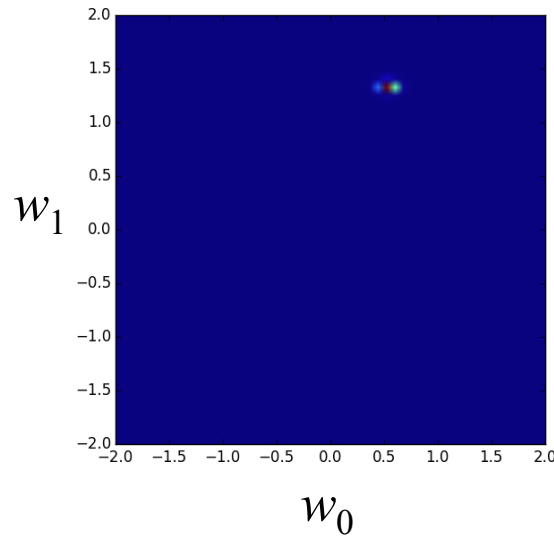
- Linear regression
- Bayesian regression models
- **Sequential Bayesian learning**

Sequential Bayesian learning

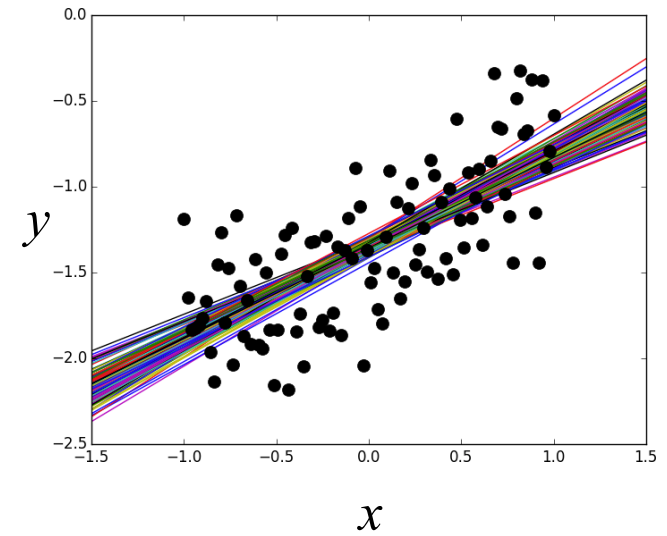
$$p(\mathbf{w})$$



$$p(\mathbf{w} \mid x, y)$$



\mathbf{w} samples in
data space (x, y)



Adapted from Carl Henrik Ek's lecture (DD2434, 2015)

Short outline for today

1. Recap from Lecture 2
2. Regression models
 - a) maximum likelihood, regularization
 - b) Bayesian approach, model selection
3. **Model selection.**

Bayesian model comparison

- Evidence framework

$$p(\mathbf{w} | \mathcal{D}) = \frac{p(\mathcal{D} | \mathbf{w})p(\mathbf{w})}{p(\mathcal{D})}$$

- The denominator does not change with \mathbf{w}

$$p(\mathbf{w} | \mathbf{t}_D, \mathbf{X}_D) \propto p(\mathbf{t}_D | \mathbf{w}, \mathbf{X}_D)p(\mathbf{w})$$

Bayesian model comparison

- Evidence framework

$$p(\mathbf{w} | \mathcal{D}) = \frac{p(\mathcal{D} | \mathbf{w})p(\mathbf{w})}{p(\mathcal{D})}$$

- The denominator does not change with \mathbf{w}

$$p(\mathbf{w} | \mathbf{t}_D, \mathbf{X}_D) \propto p(\mathbf{t}_D | \mathbf{w}, \mathbf{X}_D)p(\mathbf{w})$$

- $p(\mathcal{D})$ shows where the model spreads its probability mass over the data space (**evidence of the model**)

$$p(\mathbf{w} | \mathcal{D}, \mathcal{M}_i) = \frac{p(\mathcal{D} | \mathbf{w}, \mathcal{M}_i)p(\mathbf{w} | \mathcal{M}_i)}{p(\mathcal{D} | \mathcal{M}_i)}$$

Bayesian model comparison

- What can we do with model **evidence**?

posterior: $p(\mathcal{M}_i | \mathcal{D}) \propto p(\mathcal{M}_i) p(\mathcal{D} | \mathcal{M}_i)$

marginal likelihood

Bayesian model comparison

- What can we do with model **evidence**?

posterior: $p(\mathcal{M}_i | \mathcal{D}) \propto p(\mathcal{M}_i) p(\mathcal{D} | \mathcal{M}_i)$

- for the same priors, the posterior ratio between \mathcal{M}_1 and \mathcal{M}_2

$$\frac{p(\mathcal{D} | \mathcal{M}_1)}{p(\mathcal{D} | \mathcal{M}_2)} \quad \text{Bayes factor}$$

Bayesian model comparison

- What can we do with model **evidence**?

posterior: $p(\mathcal{M}_i | \mathcal{D}) \propto p(\mathcal{M}_i) p(\mathcal{D} | \mathcal{M}_i)$

- for the same priors, the posterior ratio between \mathcal{M}_1 and \mathcal{M}_2

$$\frac{p(\mathcal{D} | \mathcal{M}_1)}{p(\mathcal{D} | \mathcal{M}_2)} \quad \text{Bayes factor}$$

- how do we find the evidence $p(\mathcal{D} | \mathcal{M}_i)$?

$$p(\mathcal{D} | \mathcal{M}_i) = \int p(\mathcal{D} | \mathbf{w}, \mathcal{M}_i) p(\mathbf{w} | \mathcal{M}_i) d\mathbf{w}$$

Bayesian model comparison

- What can we do with model **evidence**?

posterior: $p(\mathcal{M}_i | \mathcal{D}) \propto p(\mathcal{M}_i) p(\mathcal{D} | \mathcal{M}_i)$

- for the same priors, the posterior ratio between \mathcal{M}_1 and \mathcal{M}_2

$$\frac{p(\mathcal{D} | \mathcal{M}_1)}{p(\mathcal{D} | \mathcal{M}_2)} \quad \text{Bayes factor}$$

- how do we find the evidence $p(\mathcal{D} | \mathcal{M}_i)$?

$$p(\mathcal{D} | \mathcal{M}_i) = \int p(\mathcal{D} | \mathbf{w}, \mathcal{M}_i) p(\mathbf{w} | \mathcal{M}_i) d\mathbf{w}$$

“The evidence can be seen as the probability of generating the data set from a model whose parameters are sampled at random from the prior”

Bishop, sec.3.4

Bayesian model comparison

- What can we do with model **evidence**?

posterior: $p(\mathcal{M}_i | \mathcal{D}) \propto p(\mathcal{M}_i) p(\mathcal{D} | \mathcal{M}_i)$

- prediction can be made using the “best” model (single most probable model) or can be averaged from the mixture of K models

Model mixture: $p(t | \mathbf{x}, \mathcal{D}) = \sum_{i=1}^K p(t | \mathbf{x}, \mathcal{M}_i, \mathcal{D}) p(\mathcal{M}_i | \mathcal{D})$

Bayesian model comparison

- Simple approximation for a single parameter w

$$p(\mathcal{D} | \mathcal{M}_i) = \int p(\mathcal{D} | w, \mathcal{M}_i) p(w | \mathcal{M}_i) dw$$

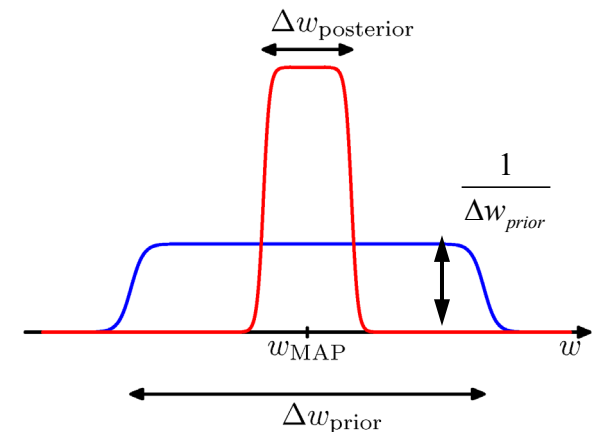
Bayesian model comparison

- Simple approximation for a single parameter w

$$p(\mathcal{D} | \mathcal{M}_i) = \int p(\mathcal{D} | w, \mathcal{M}_i) p(w | \mathcal{M}_i) dw$$

- If the *posterior* is sharply peaked around some w_{MAP} , with the width $\Delta w_{\text{posterior}}$, and the *prior* is flat with the width Δw_{prior} , then

$$p(\mathcal{D} | \mathcal{M}_i) \approx p(\mathcal{D} | w_{\text{MAP}}, \mathcal{M}_i) \frac{\Delta w_{\text{posterior}}}{\Delta w_{\text{prior}}}$$



Bayesian model comparison

- Simple approximation for a single parameter w

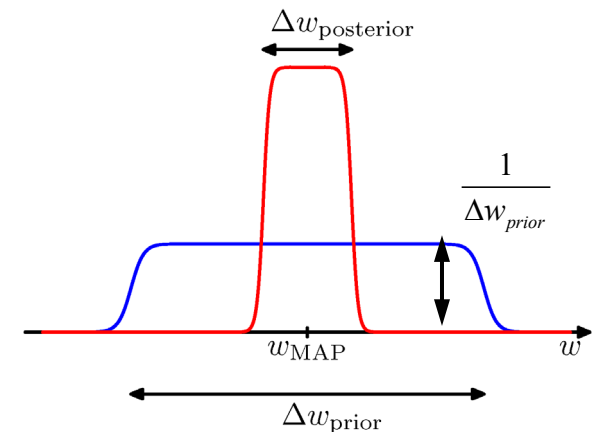
$$p(\mathcal{D} | \mathcal{M}_i) = \int p(\mathcal{D} | w, \mathcal{M}_i) p(w | \mathcal{M}_i) dw$$

- If the *posterior* is sharply peaked around some w_{MAP} , with the width $\Delta w_{\text{posterior}}$, and the *prior* is flat with the width Δw_{prior} , then

$$p(\mathcal{D} | \mathcal{M}_i) \approx p(\mathcal{D} | w_{\text{MAP}}, \mathcal{M}_i) \frac{\Delta w_{\text{posterior}}}{\Delta w_{\text{prior}}}$$



$$\ln p(\mathcal{D} | \mathcal{M}_i) \approx \ln p(\mathcal{D} | w_{\text{MAP}}, \mathcal{M}_i) + \ln \left(\frac{\Delta w_{\text{posterior}}}{\Delta w_{\text{prior}}} \right)$$



Bayesian model comparison

- Simple approximation for a single parameter w

$$p(\mathcal{D} | \mathcal{M}_i) = \int p(\mathcal{D} | w, \mathcal{M}_i) p(w | \mathcal{M}_i) dw$$

- If the posterior is sharply peaked around some w_{MAP} , with the width $\Delta w_{\text{posterior}}$, and the prior is flat with the width Δw_{prior} , then

$$p(\mathcal{D} | \mathcal{M}_i) \approx p(\mathcal{D} | w_{\text{MAP}}, \mathcal{M}_i) \frac{\Delta w_{\text{posterior}}}{\Delta w_{\text{prior}}}$$



$$\ln p(\mathcal{D} | \mathcal{M}_i) \approx \ln p(\mathcal{D} | w_{\text{MAP}}, \mathcal{M}_i) + \textcolor{red}{M} \ln \left(\frac{\Delta w_{\text{posterior}}}{\Delta w_{\text{prior}}} \right)$$

Similar estimate can be made for $\textcolor{red}{M}$ parameters (assuming their distributions behave similarly)

Bayesian model comparison

- Simple approximation for a single parameter w

$$p(\mathcal{D} | \mathcal{M}_i) = \int p(\mathcal{D} | w, \mathcal{M}_i) p(w | \mathcal{M}_i) dw$$

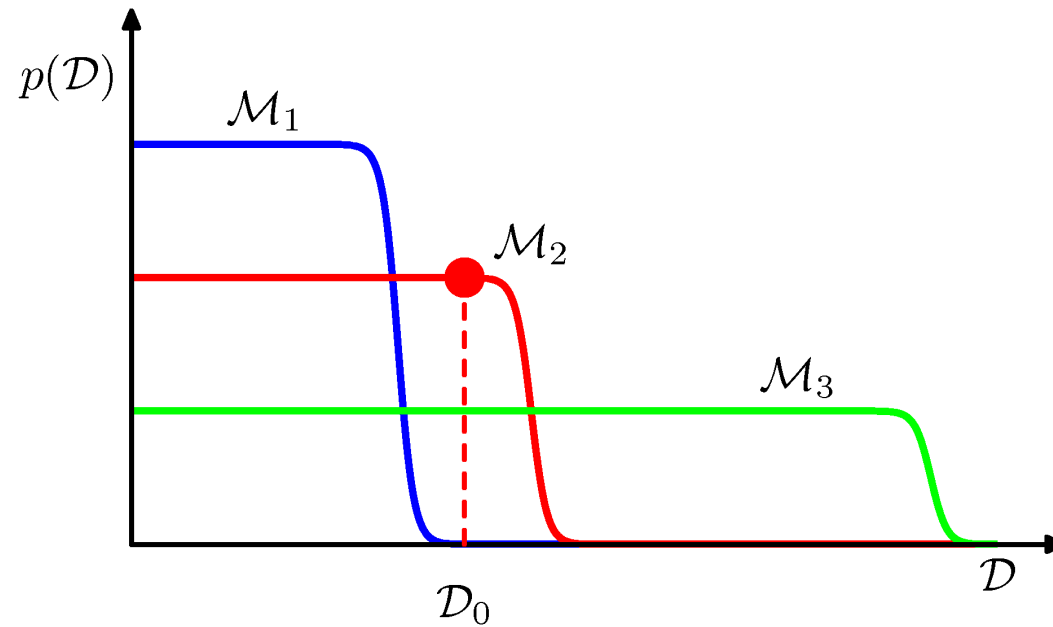
- If the posterior is sharply peaked around some w_{MAP} , with the width $\Delta w_{\text{posterior}}$, and the prior is flat with the width Δw_{prior} , then

$$p(\mathcal{D} | \mathcal{M}_i) \approx p(\mathcal{D} | w_{\text{MAP}}, \mathcal{M}_i) \frac{\Delta w_{\text{posterior}}}{\Delta w_{\text{prior}}}$$



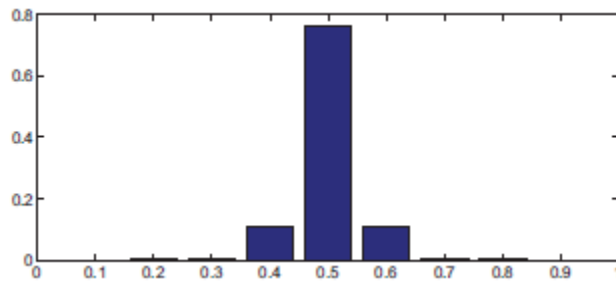
$$\ln p(\mathcal{D} | \mathcal{M}_i) \approx \ln p(\mathcal{D} | w_{\text{MAP}}, \mathcal{M}_i) + \textcolor{red}{M} \ln \left(\frac{\Delta w_{\text{posterior}}}{\Delta w_{\text{prior}}} \right) \quad \left\{ \begin{array}{l} \text{It can be seen as} \\ \textit{Occam factor.} \end{array} \right.$$

Bayesian model comparison

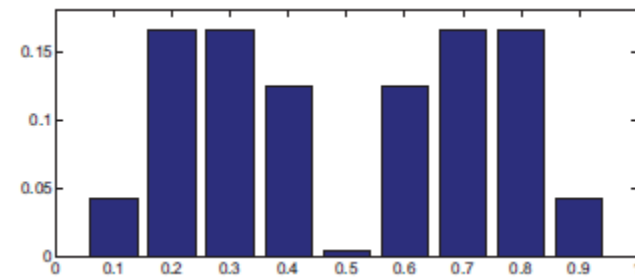


Example – a discrete parameter space

We have two discrete models: “fair” coin (M_1) and “biased” coin (M_2) model



prior for θ for “fair” coin (M_1)



prior for θ for “biased” coin (M_2)

The evidence for each model is:

$$p(\mathcal{D} | \mathcal{M}_i) = \sum_{\theta} p(\mathcal{D} | \theta, \mathcal{M}_i) p(\theta | \mathcal{M}_i)$$

Example – a discrete parameter space

Evidence for M_1 and M_2

$$p(\mathcal{D} | \mathcal{M}_i) = \sum_{\theta} p(\mathcal{D} | \theta, \mathcal{M}_i) p(\theta | \mathcal{M}_i)$$

For N_H heads and N_T tails, we obtain the following evidence for model i :

$$p(\mathcal{D} | \mathcal{M}_i) = \sum_{\theta} \theta^{N_H} (1 - \theta)^{N_T} p(\theta | \mathcal{M}_i)$$

Example – a discrete parameter space

Evidence for M_1 and M_2

$$p(\mathcal{D} | \mathcal{M}_i) = \sum_{\theta} p(\mathcal{D} | \theta, \mathcal{M}_i) p(\theta | \mathcal{M}_i)$$

For N_H heads and N_T tails, we obtain the following evidence for model i :

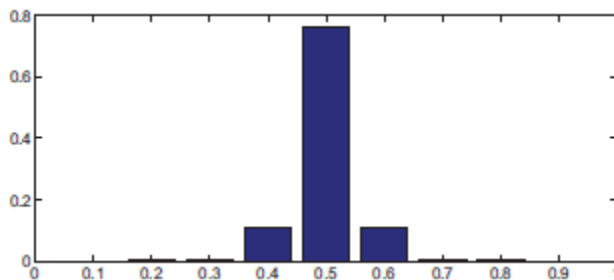
$$p(\mathcal{D} | \mathcal{M}_i) = \sum_{\theta} \theta^{N_H} (1 - \theta)^{N_T} p(\theta | \mathcal{M}_i)$$

If we assume that $p(M_1)=p(M_2)$, i.e. both “fair” & “biased” coins are equally probable, then the **Bayes’ factor** is decisive:

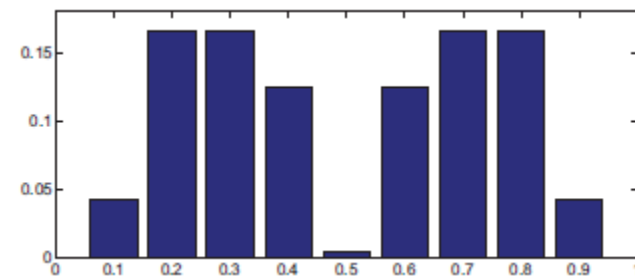
$$\frac{p(\mathcal{M}_{fair} | \mathcal{D})}{p(\mathcal{M}_{biased} | \mathcal{D})} = \frac{p(\mathcal{D} | \mathcal{M}_{fair})}{p(\mathcal{D} | \mathcal{M}_{biased})}$$

Example – a discrete parameter space

$$\theta \in \{0.1, 0.2, \dots, 0.9\}$$



prior for θ for “fair” coin (M_1)



prior for θ for “biased” coin (M_2)

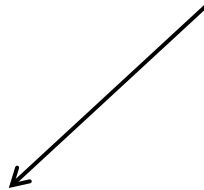
$$p(\mathcal{D} | \theta) = \theta^{N_H} (1 - \theta)^{N_T}$$

Example – a discrete parameter space

$$\theta \in \{0.1, 0.2, \dots, 0.9\}$$

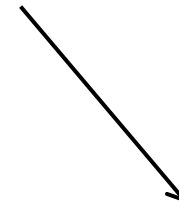
Bayes' factor estimates:

$$N_H = 5 \text{ and } N_T = 2$$



$$\frac{p(\mathcal{D} | \mathcal{M}_{fair})}{p(\mathcal{D} | \mathcal{M}_{biased})} = 1.09$$

$$N_H = 50 \text{ and } N_T = 20$$



$$\frac{p(\mathcal{D} | \mathcal{M}_{fair})}{p(\mathcal{D} | \mathcal{M}_{biased})} = 0.109$$

The evidence approximation

If hyperpriors over α and β are introduced, we obtain the predictive distribution by marginalizing out \mathbf{w} , α and β

$$p(t | \mathbf{t}, \mathbf{x}) = \iiint p(t | \mathbf{w}, \mathbf{x}, \beta) p(\mathbf{w} | \mathbf{t}, \alpha, \beta) p(\alpha, \beta | \mathbf{t}) d\mathbf{w} d\alpha d\beta$$

The evidence approximation

If hyperpriors over α and β are introduced, we obtain the predictive distribution by marginalizing out \mathbf{w} , α and β

$$p(t | \mathbf{t}, \mathbf{x}) = \iiint p(t | \mathbf{w}, \mathbf{x}, \beta) p(\mathbf{w} | \mathbf{t}, \alpha, \beta) p(\alpha, \beta | \mathbf{t}) d\mathbf{w} d\alpha d\beta$$

From Bayes theorem:

$$p(\alpha, \beta | \mathbf{t}) \propto p(\mathbf{t} | \alpha, \beta) p(\alpha) p(\beta)$$

The evidence approximation

If hyperpriors over α and β are introduced, we obtain the predictive distribution by marginalizing out \mathbf{w} , α and β

$$p(t | \mathbf{t}, \mathbf{x}) = \iiint p(t | \mathbf{w}, \mathbf{x}, \beta) p(\mathbf{w} | \mathbf{t}, \alpha, \beta) p(\alpha, \beta | \mathbf{t}) d\mathbf{w} d\alpha d\beta$$

From Bayes theorem:

$$p(\alpha, \beta | \mathbf{t}) \propto p(\mathbf{t} | \alpha, \beta) p(\alpha) p(\beta)$$

For flat prior over α and β we can resort to maximising the *marginal likelihood*.

(type II maximum likelihood)